

1-Octanol
111-87-5 | DTXSID7021940

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.84 | 0.55 | 0.85 | 0.53 | 0.83 | 0.64 |

Model Results

Predicted value: 42.3

Global applicability domain: Inside

Local applicability domain index: 5.23e-01

Confidence level: 6.39e-01

Nearest Neighbors from the Training Set

Image not found

Butyl ether

Measured: 72.4

Predicted: 32.3

Image not found

Cyclohexane

Measured: 83.2

Predicted: 59.1

Image not found

cis-Nanophine

Measured: 5.01

Predicted: 6.12

Image not found

1-Ethenoxy-2-ethylhexane

Measured: 603

Predicted: 284